CLAIMS

1. A prodrug compound having, as a modification group to be eliminated from the prodrug, a group represented by the formula:

$$\begin{array}{c} X_1 \\ Y - D_2 - D_1 - W - N \\ R \end{array}$$

formula:

wherein

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 X_1 and X_2

are each an oxygen atom or a sulfur atom,
is a chain divalent hydrocarbon group optionally having
substituent(s) or a divalent group represented by the

wherein W_1 and W_2 are each a chain divalent

$$---$$
W₁ $--$ Z $--$ W₂ $---$

hydrocarbon group or a bond, Z is a divalent hydrocarbon ring group optionally having substituent(s), a divalent heterocyclic group optionally having substituent(s), an oxygen atom, SOn wherein n is 0, 1 or 2, or >N-E wherein E is a 20 hydrogen atom, a hydrocarbon group optionally having substituent(s), a heterocyclic group optionally having substituent(s), a lower alkanoyl group, a lower alkoxycarbonyl group, an aralkyloxycarbonyl 25 group, a thiocarbamoyl group, a lower alkylsulfinyl group, a lower alkylsulfonyl group, a sulfamoyl group, a mono-lower alkylsulfamoyl group, a di-lower alkylsulfamoyl group, an arylsulfamoyl group, an arylsulfinyl group, an arylsulfonyl group, an

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arylcarbonyl group or a carbamoyl group optionally

having substituent(s), and when Z is an oxygen atom, SO_n or >N-E, W_1 and W_2 are each a chain divalent hydrocarbon group,

R is a hydrogen atom, a hydrocarbon group optionally
having substituent(s) or a heterocyclic group optionally
having substituent(s), and

R and W

may be bonded to each other when R is not a hydrogen atom,

10 D_1 and D_2

are each a bond, an oxygen atom, a sulfur atom or $>NR_1$ wherein R_1 is a hydrogen atom or a hydrocarbon group optionally having substituent(s), except for when both D_1 and D_2 are bonds, and

- is a hydrocarbon group optionally having substituent(s) or a heterocyclic group optionally having substituent(s).
- 2. The compound of claim 1, which is a compound represented by 20 the formula (I):

$$Y - D_2 \xrightarrow{X_2} D_1 - W - N$$
(I)

wherein A is a group remaining from elimination of hydrogen from a parent compound H-A of a prodrug having a group capable of bonding to a carbon atom of a modification group eliminatable from a prodrug, via a carbon-oxygen bond, a carbon-sulfur bond or a carbon-nitrogen bond, and other symbols are as defined in claim 1, or a salt thereof.

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- 3. The compound of claim 1, wherein R is a hydrocarbon group optionally having substituent(s) or a heterocyclic group optionally having substituent(s).
- 5 4. The compound of claim 1, wherein Z is a divalent hydrocarbon ring group optionally having substituent(s) or a divalent heterocyclic group optionally having substituent(s).
- 5. The compound of claim 1, wherein X_1 and X_2 are each an oxygen atom.
 - 6. The compound of claim 1, wherein D_1 and D_2 are each a bond or an oxygen atom, except for when both D_1 and D_2 are bonds.
- 15 7. The compound of claim 1, wherein W is a chain divalent hydrocarbon group optionally having substituent(s).
 - 8. The compound of claim 1, wherein W is an ethylene group.
- 20 9. The compound of claim 1, wherein R is a C_{1-6} hydrocarbon group optionally having substituent(s).
 - 10. The compound of claim 1, wherein Y is a C_{1-6} hydrocarbon group optionally having substituent(s) or a saturated
- 25 heterocyclic group optionally having substituent(s), which contains, as ring-constituting atom, 1 to 4 heteroatom(s) selected from oxygen atom, nitrogen atom and sulfur atom.
- 11. The compound of claim 1, wherein X_1 and X_2 are each an oxygen atom, D_1 and D_2 are each a bond or an oxygen atom except for when both D_1 and D_2 are bonds, W is an ethylene group, R is a C_{1-6} alkyl group, and Y is a C_{1-6} hydrocarbon group optionally having substituent(s) or a saturated oxygen-containing

heterocyclic group optionally having substituent(s), which may further contain, as ring-constituting atom, 1 to 3 heteroatom(s) selected from oxygen atom, nitrogen atom and sulfur atom.

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12. The compound of claim 1, which is a compound represented by the formula (II):

$$Y-D_2 \xrightarrow{X_2} D_1-W-N$$

$$R$$
(II)

wherein -B₁-B₂ is a group remaining from elimination of hydrogen from a pharmaceutical compound H-B₁-B₂ wherein H-B₁- is a hydroxyl group, a thiol group, an amide group or an optionally fused, nitrogen-containing heterocycle optionally having substituent(s), which is capable of bonding to a carbon atom of a modification group eliminatable from a prodrug, via a carbon-oxygen bond, a carbon-sulfur bond or a carbon-nitrogen bond, and other symbols are as defined in claim 1, or a salt thereof.

20 13. The compound of claim 12, wherein B₁ is an optionally fused, nitrogen-containing heterocyclic group optionally having substituent(s), which is capable of bonding to a carbon atom of a modification group eliminatable from a prodrug, via a carbon-nitrogen bond.

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- 14. The compound of claim 13, wherein the nitrogen-containing heterocyclic group represented by B_1 is a 5 or 6-membered aromatic heterocyclic group containing 1 to 4 nitrogens.
- 30 15. The compound of claim 14, wherein the aromatic heterocycle

in the 5 or 6-membered aromatic heterocyclic group containing 1 to 4 nitrogens, which is represented by B_1 , is imidazole, pyrrole, pyrazole, isoxazole, oxazole, thiazole or triazole.

5 16. (1) A production method of the compound of claim 2, which comprises reacting a pharmaceutical compound having an eliminatable proton (H) represented by the formula (III):

H-A (III)

or a salt thereof with a compound represented by the formula 10 (IV):

$$Y - D_2 \xrightarrow{X_2} D_1 - W - N$$

(IV)

wherein X is a leaving group, and other symbols are as defined
in claim 1, or a salt thereof, or a compound of the formula
15 (V):

$$Y-D_2 D_1 W-N = C X_1$$

(V)

wherein each symbol is as defined in claim 1, or a salt thereof.

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17. A compound represented by the formula (VI):

$$X_{2}$$
 R' X_{1}
 $Y-D_{2}'-C-D_{1}'-W'-N-C-X$

(VI)

wherein X_1 and X_2 are each an oxygen atom or a sulfur atom, W' is a chain divalent hydrocarbon group having 2 or more carbon atoms and optionally having substituent(s), or a divalent

group represented by the formula:

wherein $W_1{}'$ and $W_2{}'$ are each a chain divalent hydrocarbon group or bond, Z' is a divalent hydrocarbon ring group optionally

- having substituent(s) or a divalent heterocyclic group optionally having substituent(s), R' is a hydrocarbon group optionally having substituent(s) or a heterocyclic group optionally having substituent(s), R' is optionally bonded to W', D_1 ' is an oxygen atom or a sulfur atom and D_2 ' is an oxygen
- atom, or D_1 ' is a sulfur atom and D_2 ' is a bond, Y is a hydrocarbon group optionally having substituent(s) or a heterocyclic group optionally having substituent(s), and X is a leaving group, or a salt thereof.
- 15 18. Use of a compound represented by the formula (IV):

$$Y - D_2 \xrightarrow{X_2} D_1 - W - N$$

$$R$$

$$(IV)$$

wherein X is a leaving group, and other symbols are as defined in claim 1, for the production of a prodrug compound or a salt thereof.

19. Use of a compound of the formula (V):

$$Y - D_2 = D_1 - W - N = C = X_1$$
(V)

25 wherein each symbol is as defined in claim 1, for the production of a prodrug compound or a salt thereof.